

1-Octadecanol
112-92-5 | DTXSID8026935

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.84	0.55	0.85	0.53	0.83	0.64

Model Results

Predicted value: 1210

Global applicability domain: Outside

Local applicability domain index: 3.12e-01

Confidence level: 5.28e-01

Nearest Neighbors from the Training Set

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Hexadecane

Measured: 5010

Predicted: 3680

[Image not found](#)

Trioctylamine

Measured: 85.1

Predicted: 106

[Image not found](#)

Di(2-ethylhexyl) phthalate

Measured: 589

Predicted: 295

[Image not found](#)

Cyclododecane

Measured: 8130

Predicted: 3280